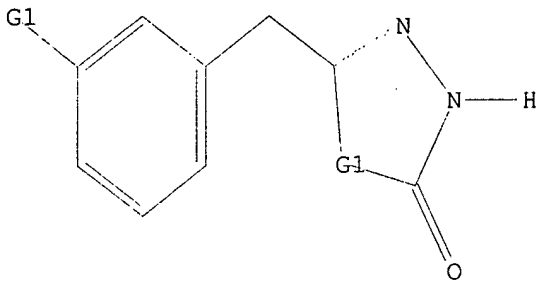
STN Structure Search (Registry/Caplus)

L3 HAS NO ANSWERS
L3 STR



G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l3 full
FULL SEARCH INITIATED 12:49:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1165 TO ITERATE

100.0% PROCESSED 1165 ITERATIONS 54 ANSWERS
SEARCH TIME: 00.00.01

L4 54 SEA SSS FUL L3

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 334.32 334.53

FILE 'CAPLUS' ENTERED AT 12:49:44 ON 27 SEP 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 27 Sep 2006 VOL 145 ISS 14
FILE LAST UPDATED: 26 Sep 2006 (20060926/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l4
L5 8 L4

L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:101011 CAPLUS
DOCUMENT NUMBER: 144:192258
TITLE: Benzyltriazolone compounds as non-nucleoside reverse transcriptase inhibitors, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Dunn, James, Patrick; Elworthy, Todd, Richard; Stefanidis, Dimitrios; Sweeney, Zachary, Kevin
PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

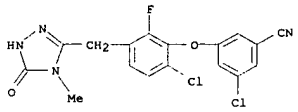
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006010545	A1	20060202	WO 2005-EP7893	20050720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006025462	A1	20060202	US 2005-190478	20050727
PRIORITY APPLN. INFO.:			US 2004-591311P P	20040727

OTHER SOURCE(S): MARPAT 144:192258
GI

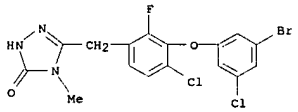
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to benzyltriazolones I, which are non-nucleoside reverse transcriptase inhibitors. In compds. I, R1 is halo, C1-6 alkyl, or C1-6 alkoxy; R2 is H, halo, or C1-6 alkyl; R3 is Ph, substituted with one to three substituents independently selected from halo, cyano, C1-6 alkyl, C1-6 haloalkyl, C1-6 haloalkoxy, and C3-8 cycloalkyl; R4 is CH2OH, CH2OC(O)CH2CH2CO2H, or CH2OC(O)-C1-6 alkyl; and R5 is H or C1-6 alkyl; including hydrates, solvates, and salts thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising a therapeutically effective amount of I with at least one pharmaceutically acceptable carrier, excipient, or diluent, as well as to the use of the compns. for treating diseases mediated by human immunodeficiency virus (HIV), such as AIDS or ARC (AIDS-Related Complex). Regioselective substitution of Et 2,3-difluoro-4-nitrophenylacetate with 3-cyano-5-difluoromethylphenol (5-step preparation from 1,3-dibromo-5-

L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
fluorobenzene given) gave II, which underwent hydrogenation, diazotization, bromination, alkylation with diethylzinc, and hydrazination
to give hydrazide III. III was added to Me isocyanate followed by cyclization, hydroxymethylation with formaldehyde, and ring opening of succinic anhydride, resulting in the formation of benzyltriazolone IV [R1 = Et; R4 = CH2OC(O)CH2CH2CO2H; R6 = CHF2]. The compds. of the invention are inhibitors of reverse transcriptase with IC50 values ranging from 7.4 nM to 1.25 μM, where compd. IV (R1 = R6 = Cl; R4 = CH2OH) expresses an IC50 value of 7.4 nM.
IT 765303-09-1P 765303-10-4P 765303-17-1P
765303-18-2P 765303-19-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzyltriazolones as non-nucleoside reverse
transcriptase inhibitors)
RN 765303-09-1 CAPLUS
CN Benzonitrile, 3-chloro-5-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]- (9CI) (CA INDEX NAME)

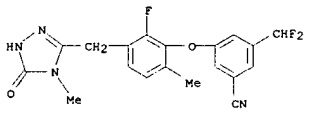


RN 765303-10-4 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[3-(3-bromo-5-chlorophenoxy)-4-chloro-2-fluorophenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

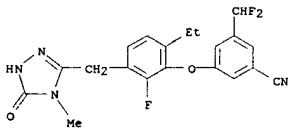


RN 765303-17-1 CAPLUS
CN Benzonitrile, 3-(difluoromethyl)-5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluoro-6-methylphenoxy]- (9CI) (CA INDEX NAME)

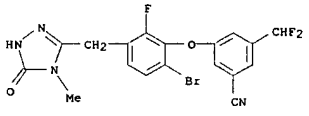
L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 765303-18-2 CAPLUS
CN Benzonitrile, 3-(difluoromethyl)-5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-6-ethyl-2-fluorophenoxy]- (9CI) (CA INDEX NAME)



RN 765303-19-3 CAPLUS
CN Benzonitrile, 3-[6-bromo-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]-5-(difluoromethyl)- (9CI) (CA INDEX NAME)

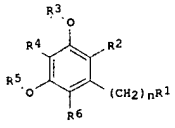


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:612072 CAPLUS
DOCUMENT NUMBER: 143:146661
TITLE: Hsp90 family protein inhibitor
INVENTOR(S): Kitamura, Yushi; Nara, Shinji; Nakagawa, Hiroshi; Nakatsu, Rieko; Nakashima, Takayuki; Soga, Shiro; Kajita, Jiro; Shiotsu, Yukimasa; Kanda, Yutaka
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: PCT Int. Appl., 311 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

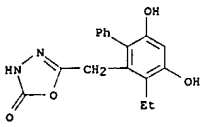
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063222	A1	20050714	WO 2004-JP19742	20041224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			JP 2003-432776 A	20031226

OTHER SOURCE(S): MARPAT 143:146661
GI

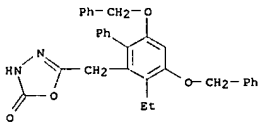


AB A Hsp90 family protein inhibitor which contains as an active ingredient a benzene derivative represented by the following general formula (I), a prodrug
thereof, or a pharmacol. acceptable salt of either.
IT 860154-88-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)
RN 860154-88-7 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-ethyl-4,6-dihydroxy[1,1'-biphenyl]-2-yl)methyl]- (9CI) (CA INDEX NAME)

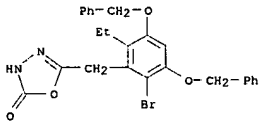
L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 860158-95-8P 860159-06-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzene derivs. as Hsp90 family protein inhibitors and antitumor agents)
RN 860158-95-8 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[[3-ethyl-4,6-bis(phenylmethoxy)[1,1'-biphenyl]-2-yl]methyl]- (9CI) (CA INDEX NAME)



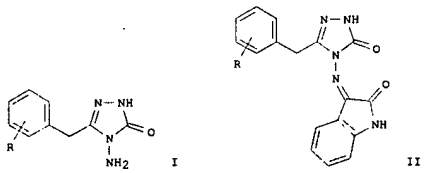
RN 860159-06-4 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[[2-bromo-6-ethyl-3,5-bis(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

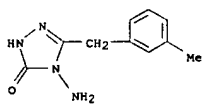
L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:318149 CAPLUS
DOCUMENT NUMBER: 144:254050
TITLE: Synthesis of 4-amino-4,5-dihydro-1H-1,2,4-triazol-5-ones and their isatin-3-imine derivatives
AUTHOR(S): Kahveci, Bahittin
CORPORATE SOURCE: Department of Chemistry, Rize Faculty of Arts and Science, Karadeniz Technical University, Rize, 53100, Turk.
SOURCE: Molecules (2005), 10(2), 376-382
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/10020376.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:254050
GI



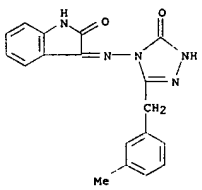
I II

AB Triazolones I (R = 2-Cl, 3-Cl, 2-Me, 3-Me) were prepared from ester (ethoxycarbonyl)hydrazones, which were obtained from imino ester hydrochlorides and H2NNHCOOEt. Condensation of I with isatin gave II (same R).
IT 877315-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4-amino-4,5-dihydro-1H-1,2,4-triazol-5-ones and their isatin-3-imine derivs.)
RN 877315-83-8 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 4-amino-2,4-dihydro-5-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



IT 877315-87-2P
RL: SPN (Synthetic preparation); PREP (Preparation)

L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(prepn. of 4-amino-4,5-dihydro-1H-1,2,4-triazol-5-ones and their isatin-3-imine derivs.)
RN 877315-87-2 CAPLUS
CN 2H-Indol-2-one, 3-[[1,5-dihydro-3-[(3-methylphenyl)methyl]-5-oxo-4H-1,2,4-triazol-4-yl]imino]-1,3-dihydro- (9CI) (CA INDEX NAME)



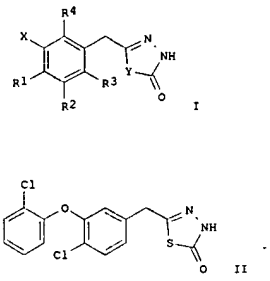
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:803934 CAPLUS
DOCUMENT NUMBER: 141:296030
TITLE: A preparation of oxadiazolone derivatives, useful as non-nucleoside reverse transcriptase inhibitors
INVENTOR(S): Dunn, James Patrick; Swallow, Steven; Sweeney, Zachary
Kevin
PATENT ASSIGNEE(S): Roche Palo Alto Llc, USA
SOURCE: U.S. Pat. Appl. Publ., 40 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Instant App.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004192704	A1	20040930	US 2004-807766	20040323
AU 2004224153	A1	20041007	AU 2004-224153	20040322
CA 2518437	AA	20041007	CA 2004-2518437	20040322
WO 2004085411	A1	20041007	WO 2004-EP2995	20040322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1608633	A1	20051228	EP 2004-722259	20040322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
BR 2004008767	A	20060328	BR 2004-8767	20040322
CN 1759104	A	20060412	CN 2004-80006480	20040322
JP 2006521319	T2	20060921	JP 2006-504792	20040322
NO 2005004264	A	20051014	NO 2005-4264	20050915
PRIORITY APPLN. INFO.:			US 2003-457130P	P 20030324
			WO 2004-EP2995	A 20040322

OTHER SOURCE(S): MARPAT 141:296030
GI



I

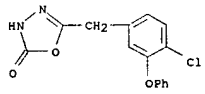
II

AB This invention relates to a preparation of oxadiazolone derivs. of formula I [wherein: X is PhO, PhS(O), PhS, PhCH2O, or indolyloxy, etc.; Y is o-phenylene, 1,2-cyclohexenylene, O, or S, etc.; R1 and R2 are independently selected from H, (halo/cyclo)alkyl, alkylthio, or haloalkoxy, etc.; R3 and R4 are independently selected from H, (halo/cyclo)alkyl, halogen, NH2, or CN, etc.] as non-nucleoside reverse transcriptase inhibitors, useful as antihiv agents. The prepared compds. were screened in HIV reverse transcriptase assay (for instance, IC50 for benzylthiadiazolone derivative II was 0.195 μM, example 22).

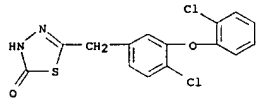
IT 765302-84-9P 765302-86-1P 765302-90-7P
765302-91-8P 765302-92-9P 765302-93-0P
765302-94-1P 765302-95-2P 765302-96-3P
765302-97-4P 765302-98-5P 765302-99-6P
765303-00-2P 765303-01-3P 765303-02-4P
765303-03-5P 765303-04-6P 765303-05-7P
765303-06-8P 765303-07-9P 765303-08-0P
765303-09-1P 765303-10-4P 765303-11-5P
765303-12-6P 765303-13-7P 765303-14-8P
765303-15-9P 765303-16-0P 765303-17-1P
765303-18-2P 765303-19-3P 765303-20-6P
765303-21-7P 765303-22-8P 765303-23-9P
765303-24-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxadiazolone derivs. useful as non-nucleoside reverse transcriptase inhibitors)

RN 765302-84-9 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(4-chloro-3-phenoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

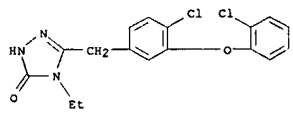
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



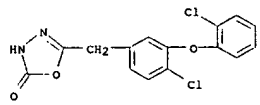
RN 765302-86-1 CAPLUS
CN 1,3,4-Thiadiazol-2(3H)-one, 5-[[4-chloro-3-(2-chlorophenoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 765302-90-7 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[4-chloro-3-(2-chlorophenoxy)phenyl]methyl]-4-ethyl-2,4-dihydro- (9CI) (CA INDEX NAME)

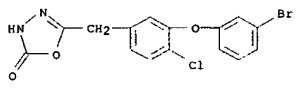


RN 765302-91-8 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[[4-chloro-3-(2-chlorophenoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

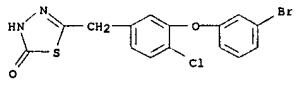


RN 765302-92-9 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[[3-(3-bromophenoxy)-4-chlorophenyl]methyl]- (9CI) (CA INDEX NAME)

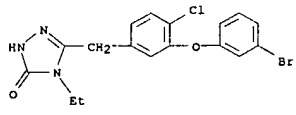
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



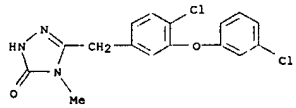
RN 765302-93-0 CAPLUS
CN 1,3,4-Thiadiazol-2(3H)-one, 5-[[3-(3-bromophenoxy)-4-chlorophenyl]methyl]- (9CI) (CA INDEX NAME)



RN 765302-94-1 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[3-(3-bromophenoxy)-4-chlorophenyl]methyl]-4-ethyl-2,4-dihydro- (9CI) (CA INDEX NAME)

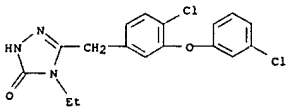


RN 765302-95-2 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[4-chloro-3-(3-chlorophenoxy)phenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

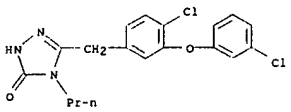


RN 765302-96-3 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[4-chloro-3-(3-chlorophenoxy)phenyl]methyl]-4-ethyl-2,4-dihydro- (9CI) (CA INDEX NAME)

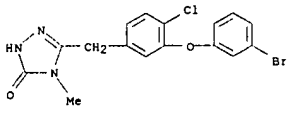
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



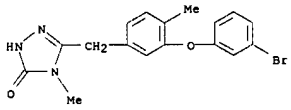
RN 765302-97-4 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[4-chloro-3-(3-chlorophenoxy)phenyl]methyl]-2,4-dihydro-4-propyl- (9CI) (CA INDEX NAME)



RN 765302-98-5 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[3-(3-bromophenoxy)-4-chlorophenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

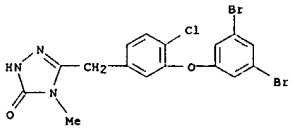


RN 765302-99-6 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[3-(3-bromophenoxy)-4-methylphenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

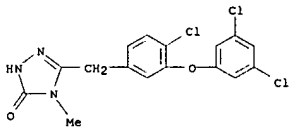


L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

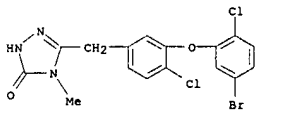
RN 765303-00-2 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[4-chloro-3-(3,5-dibromophenoxy)phenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)



RN 765303-01-3 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[4-chloro-3-(3,5-dichlorophenoxy)phenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

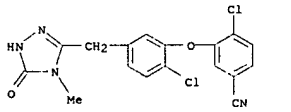


RN 765303-02-4 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[3-(5-bromo-2-chlorophenoxy)-4-chlorophenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

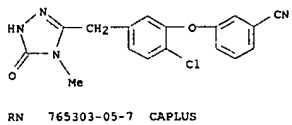


RN 765303-03-5 CAPLUS
CN Benzonitrile,
4-chloro-3-[2-chloro-5-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]phenoxy]- (9CI) (CA INDEX NAME)

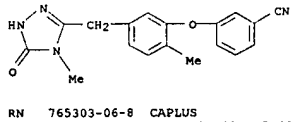
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



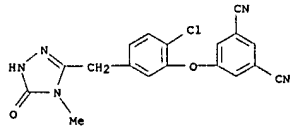
RN 765303-04-6 CAPLUS
CN Benzonitrile,
3-[2-chloro-5-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]phenoxy]- (9CI) (CA INDEX NAME)



RN 765303-05-7 CAPLUS
CN Benzonitrile, 3-[5-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

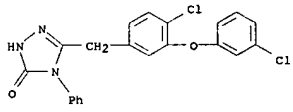


RN 765303-06-8 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[2-chloro-5-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]phenoxy]- (9CI) (CA INDEX NAME)

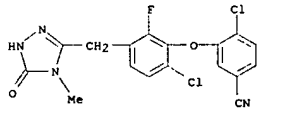


RN 765303-07-9 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[4-chloro-3-(3-chlorophenoxy)phenyl]methyl]-2,4-dihydro-4-phenyl- (9CI) (CA INDEX NAME)

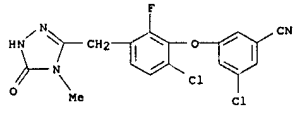
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



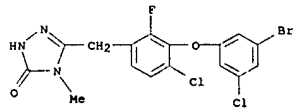
RN 765303-08-0 CAPLUS
CN Benzonitrile,
4-chloro-3-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]- (9CI) (CA INDEX NAME)



RN 765303-09-1 CAPLUS
CN Benzonitrile,
3-chloro-5-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]- (9CI) (CA INDEX NAME)

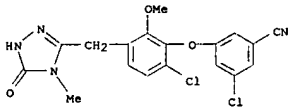


RN 765303-10-4 CAPLUS
CN 3H-1,2,4-Triazol-3-one, 5-[[3-(3-bromo-5-chlorophenoxy)-4-chloro-2-fluorophenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

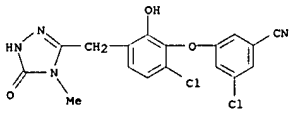


RN 765303-11-5 CAPLUS
CN Benzonitrile,
3-chloro-5-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-

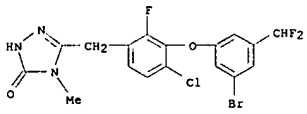
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
triazol-3-yl)methyl]-2-methoxyphenoxy]- (9CI) (CA INDEX NAME)



RN 765303-12-6 CAPLUS
CN Benzonitrile,
3-chloro-5-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-hydroxyphenoxy]- (9CI) (CA INDEX NAME)

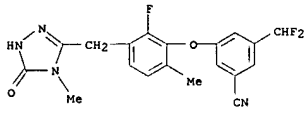


RN 765303-13-7 CAPLUS
CN 3H-1,2,4-Triazol-3-one,
5-[[3-[3-bromo-5-(difluoromethyl)phenoxy]-4-chloro-2-fluorophenyl]methyl]-2,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

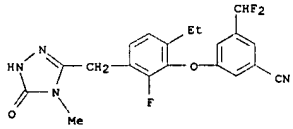


RN 765303-14-8 CAPLUS
CN Benzonitrile,
3-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]-5-(difluoromethyl)- (9CI) (CA INDEX NAME)

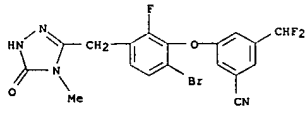
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 765303-18-2 CAPLUS
CN Benzonitrile, 3-(difluoromethyl)-5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-6-ethyl-2-fluorophenoxy]- (9CI) (CA INDEX NAME)

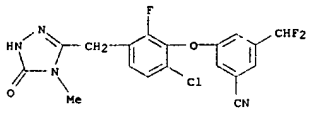


RN 765303-19-3 CAPLUS
CN Benzonitrile,
3-[6-bromo-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]-5-(difluoromethyl)- (9CI) (CA INDEX NAME)

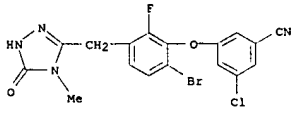


RN 765303-20-6 CAPLUS
CN Benzonitrile,
3-chloro-5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-6-ethyl-2-fluorophenoxy]- (9CI) (CA INDEX NAME)

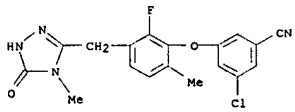
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 765303-15-9 CAPLUS
CN Benzonitrile,
3-[6-bromo-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]-5-chloro- (9CI) (CA INDEX NAME)

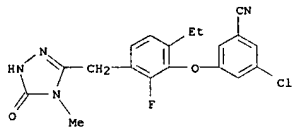


RN 765303-16-0 CAPLUS
CN Benzonitrile,
3-chloro-5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluoro-6-methylphenoxy]- (9CI) (CA INDEX NAME)

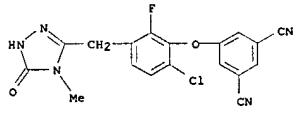


RN 765303-17-1 CAPLUS
CN Benzonitrile, 3-(difluoromethyl)-5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluoro-6-methylphenoxy]- (9CI) (CA INDEX NAME)

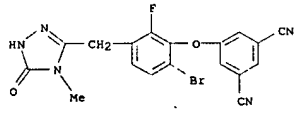
L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



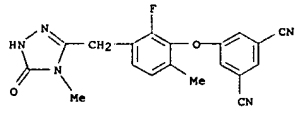
RN 765303-21-7 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[6-chloro-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]- (9CI) (CA INDEX NAME)



RN 765303-22-8 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[6-bromo-3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluorophenoxy]- (9CI) (CA INDEX NAME)

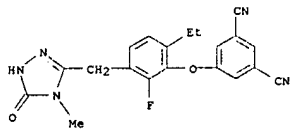


RN 765303-23-9 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-triazol-3-yl)methyl]-2-fluoro-6-methylphenoxy]- (9CI) (CA INDEX NAME)



RN 765303-24-0 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[3-[(4,5-dihydro-4-methyl-5-oxo-1H-1,2,4-

L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
triazol-3-yl)methyl]-6-ethyl-2-fluorophenoxy]- (9CI) (CA INDEX NAME)



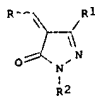
L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:101128 CAPLUS
DOCUMENT NUMBER: 134:147599
TITLE: Preparation of 2-pyrazolin-5-ones as inhibitors of serine/threonine and tyrosine kinase activity
INVENTOR(S): Moset, Marina M.; Berlanga, Jose Maria Castellano; Fernandez, Isabel F.; Calderwood, David J.; Rafferty, Paul; Arnold, Lee
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 226 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001009121	A2	20010208	WO 2000-US20628	20000728
WO 2001009121	A3	20020502		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 7060822	B1	20060613	US 2000-621468	20000724
CA 2380644	AA	20010208	CA 2000-2380644	20000728
BR 2000012896	A	20020618	BR 2000-12896	20000728
EP 1218373	A2	20020703	EP 2000-950852	20000728
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
TR 200200928	T2	20020923	TR 2002-928	20000728
JP 2003506368	T2	20030218	JP 2001-514324	20000728
NZ 516850	A	20040924	NZ 2000-516850	20000728
ZA 2002000477	A	20030422	ZA 2002-477	20020118
NO 2002000487	A	20020312	NO 2002-487	20020130
BG 106392	A	20021229	BG 2002-106392	20020206
PRIORITY APPLN. INFO.:			US 1999-146563P	P 19990730
			WO 2000-US20628	W 20000728

OTHER SOURCE(S): MARPAT 134:147599
GI

L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

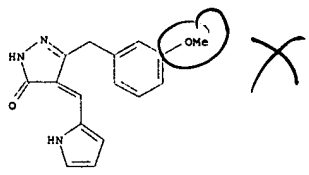


I

AB The title compds. [I; R = (un)substituted alkyl, aryl, cycloalkyl, etc.; R1 = H, AZ; R2 = H, (un)substituted alkyl, aryl, etc.; A = (CH2)n, (CH2)nNH, (CH2)nO, etc.; Z = H, alkyl, aralkyl, etc.] which are inhibitors of serine/threonine and tyrosine kinase activity, were prepared and formulated. Thus, reacting 3-cyclopropyl-2-pyrazolin-5-one with 4,5-dimethylpyrrole-2-carboxaldehyde in the presence of piperidine in EtOH afforded 30% I (R = 4,5-dimethylpyrrol-2-yl; R1 = cyclopropyl). All exemplified compds. I inhibit KDR kinase at 50 μM and some of them also significantly inhibit other PTKs such as lck at ≤ 50 μM, and cdc2 at < 50 μM. Several of the tyrosine kinases, whose activity is inhibited by the compds. I are involved in angiogenic processes. Thus, the compds. I can ameliorate disease states where angiogenesis or endothelial cell hyperproliferation is a factor. These compds. I can be used to treat cancer and hyperproliferative disorders.

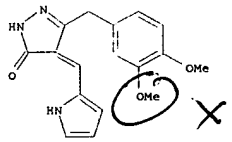
IT 324547-89-9P 324547-90-2P 324550-00-7P
324550-01-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-pyrazolin-5-ones as inhibitors of serine/threonine and tyrosine kinase activity)

RN 324547-89-9 CAPLUS
CN 3H-Pyrazol-3-one, 2,4-dihydro-5-[(3-methoxyphenyl)methyl]-4-(1H-pyrrol-2-ylmethylene)- (9CI) (CA INDEX NAME)

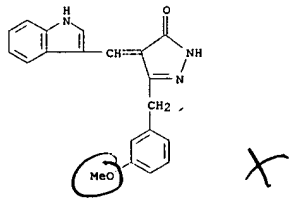


RN 324547-90-2 CAPLUS
CN 3H-Pyrazol-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-2,4-dihydro-4-(1H-pyrrol-2-ylmethylene)- (9CI) (CA INDEX NAME)

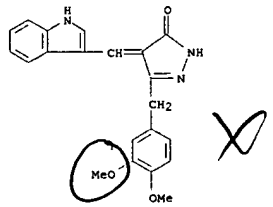
L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 324550-00-7 CAPLUS
CN 3H-Pyrazol-3-one, 2,4-dihydro-4-(1H-indol-3-ylmethylene)-5-[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

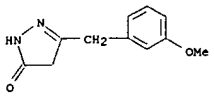


RN 324550-01-8 CAPLUS
CN 3H-Pyrazol-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-2,4-dihydro-4-(1H-indol-3-ylmethylene)- (9CI) (CA INDEX NAME)

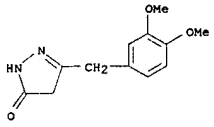


IT 324570-42-5P 324570-43-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-pyrazolin-5-ones as inhibitors of serine/threonine

L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
tyrosine kinase activity)
RN 324570-42-5 CAPLUS
CN 3H-Pyrazol-3-one, 2,4-dihydro-5-[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



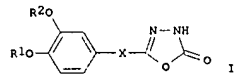
RN 324570-43-6 CAPLUS
CN 3H-Pyrazol-3-one, 5-[(3,4-dimethoxyphenyl)methyl]-2,4-dihydro- (9CI) (CA INDEX NAME)



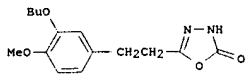
L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:380140 CAPLUS
DOCUMENT NUMBER: 122:160646
TITLE: Preparation of oxadiazole derivatives as antiasthmatics, analgesics, and inflammation inhibitors
INVENTOR(S): Soda, Takashi; Ashida, Yasuko; Doi, Takayuki; Ooi, Satoru
PATENT ASSIGNEE(S): Takeda Chemical Industries Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06192244	A2	19940712	JP 1993-274634	19931102
PRIORITY APPLN. INFO.:			JP 1992-295432 A1	19921104

OTHER SOURCE(S): MARPAT 122:160646
GI



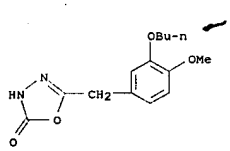
I



II

AB The title compds. I [R1 = alkyl; R2 = (un)substituted hydrocarbon; X = bond, etc.] are prepared Oxadiazole derivative II was prepared in a multiple step process starting with Me 3-(3-butoxy-4-methoxyphenyl)propionate. II at 50 mg/Kg orally gave 57.1% inhibition of carrageenin-induced edema in rats.
IT 161178-60-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxadiazole derivs. as antiasthmatics, analgesics, and inflammation inhibitors)
RN 161178-60-5 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-butoxy-4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

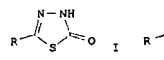
L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



L5 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:53911 CAPLUS
DOCUMENT NUMBER: 98:53911
TITLE: 1,3,4-Thiadiazolones
INVENTOR(S): Kristinsson, Haukar
PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.
SOURCE: Brit. UK Pat. Appl., 10 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

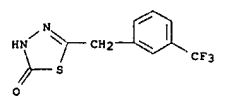
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2094791	A	19820922	GB 1982-5261	19820223
GB 2094791	B2	19850403		
US 4448968	A	19840515	US 1982-351095	19820223
DE 3206639	A1	19821104	DE 1982-3206639	19820224
PRIORITY APPLN. INFO.:			CH 1981-1336 A	19810227

OTHER SOURCE(S): MARPAT 98:53911
GI



I II

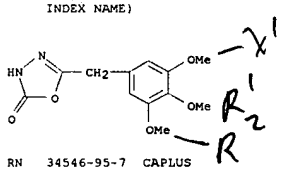
AB The insecticidal, acaricidal, fungicidal, and pharmaceutical active (no data) thiadiazolones I [R = (un)substituted C1-12 alkyl, (un)substituted C2-8-alkenyl, C3-8 cycloalkyl, NH2, alkylamino, dialkylamino, C1-6 alkoxycarbonyl, aminocarbonyl (un)substituted phenyl] were prepared via the alkoxythiadiazoles II (R1 = alkyl). Thus, o-Me thiocarbazate was cyclized with Et formimidate to give II (R = H, R1 = Me), which was demethylated by treatment with HCl to give I (R = H).
IT 84352-90-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 84352-90-9 CAPLUS
CN 1,3,4-Thiadiazol-2(3H)-one, 5-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

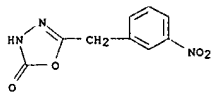
L5 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:3767 CAPLUS
DOCUMENT NUMBER: 76:3767
TITLE: 2-Benzyl-1,3,4-oxadiazolin-5-one and related compounds
AUTHOR(S): Rosen, Gerald M.; Popp, Frank D.; Gemmill, Frederick Q., Jr.
CORPORATE SOURCE: Dep. Chem., Clarkson Coll. Technol., Potsdam, NY, USA
SOURCE: Journal of Heterocyclic Chemistry (1971), 8(4), 659-62
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 4-(R-substituted)-2-benzyl-1,3,4-oxadiazolin-5-ones (I, R = H, Me, Ph, PhCH2) optionally substituted at the Ph ring, and similarly, 2-styryl-1,3,4-oxadiazolin-5-ones were prepared and acylated, reduced (with cleavage) and treated e.g. with morpholine, to give a product with morpholino group substituted at the C α to the 2-position.
IT 34546-93-5P 34546-95-7P 34547-01-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34546-93-5 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



$X^2 = O$

RN 34546-95-7 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)



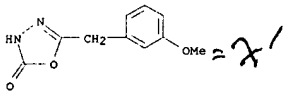
R^2 or X^1 R^1 = OMe

RN 34547-01-8 CAPLUS
CN 1,3,4-Oxadiazol-2(3H)-one, 5-[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

4-Alkoxy - not claimed

R^1, R^2

L5 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



X^1 $O\text{-}R^5$

R^5 = Me